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THEORETICAL AND EXPERIMENTAL STUDIES IN ULTRA-VIOLET SOLAR PHYSICS INCLUDING CONSTRUCTION OF LABORATORY PROTOTYPE FLIGHT EXPERIMENTS

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INTRODUCTION

The activities in theoretical and experimental research in ultraviolet solar physics have been extensive and varied in the past six months. In general, both the laboratory and theoretical activities have been directed towards important spectroscopic parameters and their connection with astrophysics. As in the past, large emphasis has been placed on the part that autoionization takes in laboratory and astrophysical plasmas. Two reports, entitled "Astrophysical Implications of Autoionization" by Professor Leo Goldberg and "Autoionization Effects in Ultraviolet Absorption Spectra of Hot Gases" by Professor W.R.S. Garton,provide a comprehensive treatment of this subject in both the laboratory and in astronomy. These reports, which have been appended, are pre-publication versions of invited papers presented at the Auto-ionization Conference at Goddard Space Flight Center in August 1965.

It became clear during the year that a solar rocket spectroscopic experiment is required to answer a number of questions which have arisen from the laboratory and theoretical research. With this background and aim in mind, Ball Brothers Research Corporation and Mr. William Fastie of Johns Hopkins University were asked to prepare for Harvard College Observatory a preliminary design of a rocket-borne spectrometer system to cover the wavelength range 1400 - 2000 Å with high spectral and/or spatial resolution. This preliminary design has been completed during the current year. In addition to initiating a Harvard Observatory rocket program, we have undertaken some cooperative research with the rocket group at Culham, Abingdon, England. Dr. Wilson and his colleagues have provided us with an original rocket spectrogram which was taken from Woomera, Australia. This spectrum is of integrated light from the solar disk and covers the wavelength region 3000 Å down to Lyman-α. We are able to carry out a detailed identification of the spectral features with our laboratory shock tube source.

In the following report, our progress in basic research will be described in detail under the sections "Instrumentation", "Theoretical Activities", "Atomic Spectroscopy" and "Molecular Spectroscopy".

INSTRUMENTATION

The fourth shock tube has been assembled and completely tested over the working range of high pressure and vacuum. Spectroscopic tests with this tube were made by recording the time integrated emission spectra in the visible region of shock-heated mixtures of trichlorosilane in argon. The line reversal temperature equipment and the pressure gauges have been added. The optical components which combine the shock tube light source with the Fabry-Perot and spectrometer have been positioned and test-runs carried out with the complete system.

A pair of glass plates with silver and magnesium fluoride coats have been obtained and aligned in the Fabry-Perot interferometer. The new plates give a finesse of at least 16 and possess the proper thermal expansion coefficient to match the barium titanate crystal. The electronics for the Fabry-Perot are working and a modification to the oscilloscope has permitted the scanning rate of the device to be decreased so that the number of photons per unit resolution have increased.

Since the testing and assembly of this experiment have now been completed we anticipate that Dr. Richard Day will commence a detailed study and scan of Stark broadened silicon lines early in the next report period.

Dr. Martin Huber has continued to prepare the experiment for the hook method which uses a Mach-Zehnder interferometer and Littrow spectrograph. Although we are not yet satisfied with the Littrow lens and expect to replace it with a higher quality optic we have been able to successfully combine both interferometer and spectrograph with the shock tube test section. Preliminary spectra have shown fringes of excellent contrast.

The final report which describes the preliminary design specifications for a rocket-borne spectrometer by the Ball Brothers Research Corporation has been appended. The original specifications and aim of the design study required a rocket-borne spectrometer system which was capable of detecting and telemetering to the ground solar radiation intensities within the range 1400 - 2000 Å while scanning the solar disc from center to limb or while pointing at the center of the sun. As design goals we required 0.01 Å spectral resolution, 1 arc minute spatial resolution and 1 % photometric accuracy. The design also includes considerations for in-flight changes of spectral scan rate and slit widths.

The study began in September 1965, and Mr. William Fastie was retained by Ball Brothers Research Corporation to carry out the optical design and advise on other optical problems in the spectrometer.

The rocket study has been reviewed. We have discussed it with other researchers at the Observatory and have decided to carry out two flights in the coming year: (1) a rocket spectrometer which will point to the center of the sun and scan from 1500 - 1950 Å with a spectral resolution of at least 0.05Å; (2) a spectrometer which will scan from the center to the limb of the sun with a spatial resolution of 5 arc seconds, a wavelength resolution in the range 1.0 - 0.1 Å and wavelength coverage from 1500 - 1850 Å. As will be indicated in the following sections, the choice and urgency of the rocket program has arisen from very recent work on the CO molecular spectrum and Si continuous absorption in the 1500 - 1700 Å region.

THEORETICAL ACTIVITIES

As interest grows in the absorption coefficient for autoionizing transitions, and, more generally, the rate coefficients for processes that involve doubly excited resonance levels of atoms, it becomes more important to understand the mechanism of resonance processes in atoms. Various workers have turned to the formal theory of scattering for descriptions of electron scattering resonances.

Mrs. B. Adams has been engaged in an attempt to generalize existing close coupling calculations to many-electron atoms. These calculations have been very successfully used by Dr. P. Burke and co-workers in predicting resonances in helium. Dr. Burke has been collaborating on these modifications, which are primarily to include magnesium and calcium.

During the last six month period, Dr. Shore has developed an approach to the theory of resonance attenuation, particularly photon attentuation, from scattering theory. This approach draws out the physical significance of observed "transmission windows" as well as the more usual Lorentz profile. The full implications of these results are now being investigated.

In particular, it is hoped that we can obtain a simple prescription for calculating autoionizing line profiles of complex atoms.

The theoretical behavior of the solar autoionization doublet of Al I at 1934 Å was investigated by Dr. G. Withbroe. The observed profile of this doublet can be explained reasonably well under the assumption of local thermodynamic equilibrium by using a classical photospheric model in which the electron temperature decreases monotonically with decreasing optical depth. Calculations made with models containing a temperature minimum indicate that the Al I autoionization lines may develop strong emission cores at the solar limb. These results suggest that it might be worthwhile to obtain center-limb observations of these lines.

Mrs. A. Dupree has calculated the strength of autoionizing lines of Ca I for stars along the spectral sequence. The behavior of these lines, the multiplet at 6350 (3d4p $^3F_4$ - 3d4d $^3G_5$), can be predicted as a function of spectral type and luminosity classification in order to confirm line strength measurements in observed stars. The theoretical strengths also allow one to select late type (MO and later), super giant and giant stars as those most favorable for identification of calcium autoionizing lines.

In addition to autoionization, work has been carried out on the chemical abundances in the solar corona by A. Dupree. She has analyzed the effects of gravitational diffusion of heavy elements in present solar winds. It appears that ions heavier than hydrogen will not partake of coronal expansion at the hydrogen expansion velocity. The differences in predicted expansion velocities among heavy ions are not systematically dependent upon the atomic weight of the element. Therefore, it does not seem possible to attribute an overabundance of elements that vary with mass to the presence of gravitational diffusion.

The observed center-limb variation of solar C_2, CO, CN and CH lines has been interpreted by Dr. Withbroe with five photospheric models. The observations are best explained by a three stream inhomogeneous model. This indicates that inhomogeneities may be important in the upper photosphere where the molecular lines are formed, $-2.5 \leq \log \tau_{5000} \leq -0.5$.

Mr. John Allen, in collaboration with Dr. Stephen Strom, has performed a preliminary study of non-thermal photospheric velocities with the multiplet method. These studies have indicated the necessity of carefully defining the mean optical depth at which a given portion of a Fraunhofer line is formed. This work was reported at the December 1965 AAS meeting in Berkeley.

In addition, Mr. Allen has carried out calculations of ionization equilibria for oxygen. These include processes of collisional ionization, radiative recombination and dielectronic recombination. The effects of including dielectronic recombination in the calculations have been discussed. Scientific Report # 7, entitled "Calculations of Ionization Equilibrium for Oxygen", describes this work. The report is appended.

A theoretical study of the ionization rates in the shock tube has also been undertaken by Mr. G. Newsom. This treatment has led to the conclusion that collisional ionization from excited levels dominates the ionization rate for temperatures near 5000°K. At 4000°K, photoionization from excited levels by photons emitted by the shock becomes comparable to collisional ionization, although both rates are much less than photoionization caused by the coaxial flash tube discharge. This discharge is estimated to upset the equilibrium electron population by several percent at 4000°K. The heating generated in the shock by the flash tube discharge is found to be negligible at 5000°K, but a small amount of heating occurs at 4000°K. These results agree with the experiment by Garton, Parkinson and Reeves, which showed equality of excitation and electron temperatures in a shock tube for temperatures from 5800° to 6800°K.

In preparation for the experimental study of Stark broadened lines in a shock tube with a Fabry-Perot, Dr. R. Day is writing a program which will generate line profiles of Stark broadened lines. The preliminary work of obtaining correlation coefficients has been performed, and the profiles are limited to about 0.5% accuracy through inaccuracies in the numerical integration techniques. Preliminary results have already indicated that the asymmetry of Stark broadened lines is larger than previously realized.

In addition, a versatile computer program for calculating profiles of atomic and molecular lines for model atmospheres has been developed by Dr. Withbroe. This program can handle up to twenty spectral lines simultaneously and permits the use of a depth-dependent microturbulence and macroturbulence.

In the past six months, a computer program has been written by Mr. John Rich and Mrs. J. Flagg which performs the calculation of chemical and ionization equilibrium behind a shock wave. When given the measured thermodynamic parameters of temperature and pressure, the program calculates the number of atoms, ions, molecules and electrons in equilibrium.

ATOMIC SPECTROSCOPY

Drs. Parkinson and Reeves, in collaboration with other scientists in the laboratory and with Professor W.R.S. Garton from Imperial College, have continued the work on atomic spectroscopy. The measurements of Al have been extended to include, with the autoionized doublet, the cross sections in the ionization continuum. An account of these measurements in Al was presented at the AAS meeting in August. In collaboration with Professor Garton, the absorption spectrum of shock-heated indium vapour has been photographed and the missing member of the sixth line group ($^2P_{\frac{1}{2},\frac{3}{2}}$ - sp^2 ^2S, ^2P) identified at 1824 Å. The sp^2 configuration and the series perturbation in indium have been carefully reviewed and the term sp^2 ^2D confirmed as the perturber of the ^2D series. The work on the indium spectrum has been submitted for publication and a scientific report, # 9, has been appended.

The absorption spectra of thallium vapour has also been recorded using the shock tube method. At the temperatures available with this source the 6 $^2P_{\frac{3}{2}}$ level was populated sufficiently for absorption lines starting on it to be recorded. The 6 $^2P_{\frac{3}{2}}$ - $6s6p^2$ $^2S_{\frac{1}{2}}$ and its companion 6 $^2P_{\frac{1}{2}}$ - $6s6p^2$ $^2S_{\frac{1}{2}}$ were photographed and identified at λ1449 and 1302 Å, respectively.

During the same investigation, the Tl vapour was also examined with a one-meter scanning vacuum spectrometer and furnace. With the resolution available in this instrument, it was possible to obtain a good line profile of the Tl 2007 autoionized line. These observations were treated according to the Fano-Beutler description of autoionization to a single continuum.

A plot of the course of the absorption coefficient for this line was also obtained and made relative to the absolute cross-sections reported by D.V. Marr and R. Heppinstall (Proc. Phys. Soc. 1966) who carried out similar measurements with somewhat lower resolution.

In conjunction with his work in the shock tube and solar spectrum, Mr. Gerald Newsom has examined Ca in a furnace and in an arc. The absorption spectrum of calcium vapor was scanned photoelectrically in the vacuum ultraviolet to yield accurate photoionization cross-sections from 1660 Å to the principal series limit. Seven new energy levels were discovered and classified in this region, and several previously known levels have been reclassified. All autoionizing transitions from the ground state expected within 300 Å of the principal series limit have now been observed. Oscillator strengths and half-widths of seven of the autoionizing lines have been measured. This work is reported in detail in the appended report, # 5, and has been submitted to Proc. Phys. Soc. for publication. 3/11/66

Arc spectra of calcium are presently being taken to obtain improved profiles of the autoionizing multiplet at 6360 Å and to attempt identification of several unidentified absorption features seen in a shock tube.

The data on simultaneously measured Fe and Cr oscillator strengths, accumulated by Drs. M. Huber and F.L. Tobey, have been further reduced by Dr. Huber. In addition to the previously reported three Cr I and six Fe I gf-values, oscillator strengths were obtained for two Cr I, three Cr II and 35 Fe I lines. Since the plates were taken with a wide slit integrating over the line profile, these lines had to be carefully selected: the plates were searched for features of appropriate strength, which, however, could be used only if they were established as lines free of blends within the spectral range of the slit width. A copy of the galley proof of the second revision of Rowland's Preliminary Table of Solar Spectrum Wavelengths (to be issued as NBS Monograph 61) proved to be of great help for this tedious task.

It was realized that the correction of the f-values due to emission from the shock could only be determined experimentally. Several new plates, therefore, were taken, which allow a separation of the light emitted and absorbed by the shock-heated gas. This was accomplished by photographing the shock emission, after the photographic emulsion had been exposed to a pure continuum flash and, thus, a point on the characteristic curve was reached which readily allowed a comparison with shock absorption spectra taken on the same plate. It was found that emission made the absorption lines to appear roughly 25% less deep than they would be without emission.

Drs. Huber and Withbroe are examining the feasibility of using the spectral region between 3000 and 4000 Å for obtaining solar abundances. The preliminary results indicate that one can obtain surprisingly reliable equivalent widths of lines in this spectral region. The results also indicate that the Fe I f-values, determined in the shock tube, are superior to existing published values.

Dr. Dorothy W. Weeks has continued work on the wavelength measurements and analysis of the iron spectrum and has extended her investigation to cover the region 3100 - 1450 Å.

Approximately 350 new lines in the vacuum ultraviolet, common to both furnace and shock tube plates, have been measured. These lines are below 2000 Å where formerly there were less than 50. From these new lines, measured on a Zeiss Comparator, 21 energy levels from 50,600 to 55,000 wave numbers have been found. The new levels classify in addition to the 49 lines, from which the levels were determined, at least 209 lines. Of these, 59 lines were previously observed in the laboratory, and an additional 174 lines were observed in the solar spectrum, 54 of which had not been identified. For more than 100 of these lines the difference between the observed and calculated wavelengths was equal to or less than 0.010 Å. These results were reported at a meeting of the American Astronomical Society in early August 1965.

Twelve additional plates have since been taken with the shock tube to provide spectrograms from 3000 - 1450 Å. This range was subdivided into three regions, 3000 - 2400 Å, 2550 - 1950 Å and 2050 - 1450 Å. Except for two exposures with iron sulphide, a mixture of $Fe(CO)_5$ and argon was used in the shock tube.

The automatic comparator at the Argonne National Laboratories has been used to help in the reduction of some of these plates. The program used at Argonne did not print out the dispersion for each standard used and required two runs on the computer to give wavelengths and wave numbers. However, a program developed by Mr. Tech at Harvard College Observatory will give the dispersion for each standard across the plate, the standard deviation, the probable error, a plot of the residuals, the wavelengths and wave numbers. Each trial for determining the polynomial that best fits the data is recorded. This program is being used for the measurements taken at Argonne. It has been used to study the region from 3003.91 - 2712.460 Å with 34 internal Fe I standards. The dispersions of this region of the plate varied from 2.74844 - 2.76136 Å/mm. For this region of 300 Å with 218 lines, the standard deviation for the standard lines is .0018 Å with a probable error of .0012 Å. No residual was greater than 0.0035 Å, indicating that the measurements agreed with the adopted values to ±1 micron. Twenty-nine of these standards were sharp lines, neither very intense nor faint. One hundred and forty-three of the 218 lines measured were previously known Fe lines. Since the Zeiss comparator used in the preliminary study measured to one micron and the Argonne comparator to 1/2 micron, that is, to 0.003 Å for the Zeiss and to 0.0015 Å for the Argonne, more precise measurements cannot be expected with the three-meter spectrograph used in this experiment.

It is planned to continue this type of study of all the plates measured at Argonne.

The problem of standards is a basic and critical one. Internal Fe I standards can be used from 2084 Å and higher. Below 2084 Å there are no secondary Fe I standards. There is a limited number of Fe I lines to 1855 Å. It will be necessary to experiment with different standards. Before resuming the determination of new energy levels, a list of precisely measured Fe I lines from 3000 Å to lower wavelengths should be compiled. This is in process.

The spectral line reversal method which is routinely used to determine the population temperature within the shock waves has been recently applied by Garton, Parkinson and Reeves to make simultaneous measurements on normal bound-bound Ca I lines and lines involving strongly autoionizing levels. The agreement of the two sets of measured temperatures identifies the electron temperature with the temperature characterizing populations of the bound excited states giving improved confidence in the existence of local thermodynamic equilibrium in the reflected shock. This work has been described in report # 8, which has been appended and has been submitted for publication. Since the gas of the shock wave is in thermodynamic equilibrium and measurements can be made of the temperature and optical depth of the shock, an experiment is now under way which will test the use of the shock radiation as an absolute standard of intensity. This work is progressing well and should be completed early in the next report period.

Mr. John Rich has continued in his laboratory and theoretical work to explain and describe the temperature minimum in the sun. In addition to his work on the carbon monoxide molecule Mr. Rich has found indications that one would have to consider bound-free metal absorption as a process competing with the absorption by CO. Rough approximations indicated that neutral Si and neutral Mg would be important in this wavelength region. For Mg, experimental data was available, but there was no experimental information on the Si atom. The bound-free absorption coefficient of neutral Si was measured in the laboratory using shock tube techniques. The absorption coefficient was measured for the ground state and for the first excited state of Si, and these observations indicated that the measured cross-sections are almost a factor of 10 higher than those originally predicted.

The results of these experiments have been included in a solar flux calculation which produced very encouraging results, and these observations were presented to the American Astronomical Society in December 1965.

MOLECULAR SPECTROSCOPY

The experimental measurements by Mr. Rich of the absorption strength of the carbon monoxide fourth-positive band system continues in the laboratory. After the initial work with the one-meter vacuum spectrograph, a complete set of calibrated plates have been taken, using a stainless steel shock tube and a three-meter vacuum spectrograph with a dispersion of about 3Å/mm. These plates cover a wavelength region between 1500 and 2000 Å. The carbon monoxide was shock-heated to temperatures varying between 4000 and 6000°K. All measurements were made in absorption. These experiments represent very good measurements, but are limited by resolution and impurity difficulties. The resolution problem is inherent with shock tube absorption measurements. Data reduction to date has only been superficial. Complete data reduction is awaiting the installation of a densitometer. Additional experimental CO cross-section measurements are not planned.

The Culham rocket spectrogram has been partially analyzed by using the technique of directly comparing spectral features in it with shock tube spectra. For this purpose a large number of molecular and atomic spectra have been taken.

These include the diatomic molecule CO, CS, OH, O_2, NO, MgO, MgH and SiO as well as the atomic spectra of Fe, Cr, Si, Mg, Na, C, and S. At the present time, diatomic bands of CO and OH, lines of Fe, Cr, Si, Mg, C and S have been identified.

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